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Magnetic anisotropy of cyclopropane and epoxide rings

Aminova R., Samitov Y.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

MO LCAO results are presented for the interatomic contribution to the anisotropy of the diamagnetic susceptibility; values of δχd=-23.5 · 10-6 and δχd=-13.8 · 10-6 cm3/mole are obtained for the cyclopropane and epoxide ring systems, respectively. The results are used to interpret PMR spectra in terms of the configuration and conformation of the α and B forms of caran-4-ol and two stereoisomers of caranone. © 1967 The Faraday Press, Inc.

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